

FILE 'USPATFULL' ENTERED AT 16:02:33 ON 04 APR 2005

L1 1 S (PROTEIN (P) HYDROPHOBICITY (P) NORMALIZE?)/CLM

L2 27 S (PROTEIN (P) HYDROPHOBICITY (P) NORMALIZE?)

L3 2 S PROTEIN (P) (HYDROPHOBICITY (3A) NORMALIZE?)

L4 3 S PROTEIN (P) (HYDROPHOBICITY (5A) NORMALIZE?)

L5 1 S L4 NOT L3

FILE 'CAPLUS' ENTERED AT 16:06:39 ON 04 APR 2005

L6 1 S PROTEIN AND (HYDROPHOBICITY (5A) NORMALIZE?)

L7 2 S (PROTEIN OR POLYPEPTIDE OR PEPTIDE) AND (HYDROPHOBICITY (5A)

L8 14 S PROTEIN AND (TOTAL HYDROPHOBICITY)

=> d bib,kwic 1-14

L8 ANSWER 1 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

AN 2004:385131 CAPLUS

DN 141:65829

TI A note on clustering the functionally-related paralogues and orthologues of **proteins**: a case of the FK506-binding **proteins** (FKBPs)

AU Galat, Andrzej

CS Departement d'Ingenierie et d'Etudes des Proteines, DSV/CEA, CEA-Saclay, Gif-sur-Yvette, F-91191, Fr.

SO Computational Biology and Chemistry (2004), 28(2), 129-140

CODEN: CBCOCH; ISSN: 1476-9271

PB Elsevier Science Ireland Ltd.

DT Journal

LA English

RE.CNT 44 THERE ARE 44 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI A note on clustering the functionally-related paralogues and orthologues of **proteins**: a case of the FK506-binding **proteins** (FKBPs)

AB The expression patterns of 18 FK506-binding **proteins** (FKBPs) encoded in the human genome have been established whereas the functional significance of the numerous ORFs coding for FKBP-like sequences remains unknown. Nominal masses of the human FKBP-like sequences vary from 12 to 135 kDa. Some large FKBP-like sequences consist up to four repeats of the 12 kDa FK506-like binding domain (FKBD) whereas other large FKBP-like sequences contain one FKBD linked to different functional domains such as TPRs, leucine-zipper, calmodulin-binding domain etc. The genomes of other eukaryotic organisms, namely *D. melanogaster*, *C. elegans*, *A. thaliana*, *S. pombe* and *S. cerevisiae* encode different nos. of the FKBP-like sequences some of which are orthologues to the human FKBP-like sequences. A library of novel algorithms was developed and used for computation of the level of conservation of the hydrophobicity and bulkiness profiles, and the amino acid compns. (AACs) of 247 aligned sequences of FKBP-like sequences. The pairwise-compared hydrophobicity and bulkiness profiles for some combinations of the aligned sequences of the FKBDs yielded high values of the correlation coeffs. (CCF). The AACs of some combinations of the aligned sequences of the FKBDs also differed to a low degree. The functionally-related orthologues and paralogues of the FKBP-like sequences were clustered by using the following criteria: 1° apparent conservation of the crucial amino acid (AA) residues for peptidylprolyl cis/trans isomerase (PPIase) activity and binding of some immunosuppressive drugs; 2° convergence of the three mentioned above properties of the polypeptide chain; 3° similarity in the sequence attributes pI and **total hydrophobicity** index (HI). The clustering method was used for setting up several hypotheses on the emergence of certain classes of the FKBP-like sequences in the eukaryotic kingdom.

ST FK506 binding **protein** clustering algorithm

IT Immunophilins

RL: BSU (Biological study, unclassified); BIOL (Biological study) (FKBP (FK 506-binding **protein**); clustering the functionally-related paralogues and orthologues of **proteins** and a case of the FK506-binding **proteins** (FKBPs))

IT Algorithm

Arabidopsis thaliana

Bioinformatics
Caenorhabditis elegans
Cluster analysis
Databases
Drosophila melanogaster
Genome
Human
Immunosuppressants
Repeat motifs (**protein**)
Saccharomyces cerevisiae
Schizosaccharomyces pombe
Sequence homology analysis
(clustering the functionally-related paralogues and orthologues of
proteins and a case of the FK506-binding **proteins**
(FKBPs))

IT Information systems
(searching; clustering the functionally-related paralogues and
orthologues of **proteins** and a case of the FK506-binding
proteins (FKBPs))
IT 95076-93-0, Peptidylprolyl cis/trans isomerase
RL: BSU (Biological study, unclassified); BIOL (Biological study)
(clustering the functionally-related paralogues and orthologues of
proteins and a case of the FK506-binding **proteins**
(FKBPs))

L8 ANSWER 2 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:813331 CAPLUS
DN 134:111900
TI On hydrophobicity correlations in **protein** chains
AU Irback, Anders; Sandelin, Erik
CS Complex Systems Division, Department of Theoretical Physics, Lund
University, Lund, S-223 62, Swed.
SO Biophysical Journal (2000), 79(5), 2252-2258
CODEN: BIOJAU; ISSN: 0006-3495
PB Biophysical Society
DT Journal
LA English

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD
ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI On hydrophobicity correlations in **protein** chains
AB We study the statistical properties of hydrophobic/polar model sequences
with unique native states on the square lattice. It is shown that this
ensemble of sequences differs from random sequences in significant ways in
terms of both the distribution of hydrophobicity along the chains and
total hydrophobicity. Whenever statistically feasible,
the analogous calcns. are performed for a set of real enzymes, too.
ST **protein** enzyme hydrophobicity model
IT Hydrophobicity
Simulation and Modeling, biological
(hydrophobicity correlations in **protein** chains)
IT Enzymes, properties
Proteins, general, properties
RL: PEP (Physical, engineering or chemical process); PRP (Properties);
PROC (Process)
(hydrophobicity correlations in **protein** chains)

L8 ANSWER 3 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 2000:761054 CAPLUS
DN 134:82374
TI On hydrophobicity correlations in **protein** chains
AU Irback, Anders; Sandelin, Erik
CS Complex Systems Division, Department of Theoretical Physics, University of
Lund, Lund, S-223 62, Swed.
SO Los Alamos National Laboratory, Preprint Archive, Condensed Matter (2000)
1-17, arXiv:cond-mat/0010390, 25 Oct 2000
CODEN: LNCMFR
URL: <http://xxx.lanl.gov/pdf/cond-mat/0010390>
PB Los Alamos National Laboratory

DT Preprint

LA English

RE.CNT 30 THERE ARE 30 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI On hydrophobicity correlations in **protein** chains

AB We study the statistical properties of hydrophobic/polar model sequences with unique native states on the square lattice. It is shown that this ensemble of sequences differs from random sequences in significant ways in terms of both the distribution of hydrophobicity along the chains and **total hydrophobicity**. Whenever statistically feasible, the analogous calcs. are performed for a set of real enzymes, too.

ST **protein** sequence analysis hydrophobicity correlations

IT Enzymes, biological studies

Proteins, general, biological studies

RL: BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study)

(hydrophobicity correlations in **protein** chains)

IT **Protein** sequence analysis

(minimal two-dimensional HP (hydrophobic/polar) model; hydrophobicity correlations in **protein** chains)

L8 ANSWER 4 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1998:638992 CAPLUS

DN 129:328067

TI Transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution

AU Harley, Carol A.; Holt, Jonathan A.; Turner, Rhiannon; Tipper, Donald J.

CS Department of Molecular Genetics and Microbiology, University of Massachusetts Medical School, Worcester, MA, 01655, USA

SO Journal of Biological Chemistry (1998), 273(38), 24963-24971

CODEN: JBCHA3; ISSN: 0021-9258

PB American Society for Biochemistry and Molecular Biology

DT Journal

LA English

RE.CNT 38 THERE ARE 38 CITED REFERENCES AVAILABLE FOR THIS RECORD

ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI Transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution

AB The determinants of transmembrane **protein** insertion orientation at the endoplasmic reticulum have been investigated in *Saccharomyces cerevisiae* using variants of a Type III (naturally exofacial N terminus (Nexo)) transmembrane fusion **protein** derived from the N terminus of Ste2p, the α -factor receptor. Small pos. and neg. charges adjacent to the transmembrane segment had equal and opposite effects on orientation, and this effect was independent of N- or C-terminal location, consistent with a purely electrostatic interaction with response mechanisms. A 3:1 bias toward Nexo insertion, observed in the absence of a charge difference, was shown to reflect the Nexo bias conferred by longer transmembrane segments. Orientation correlated best with **total hydrophobicity** rather than length, but it was also strongly affected by the distribution of hydrophobicity within the transmembrane segment. The most hydrophobic terminus was preferentially translocated. Insertion orientation thus depends on integration of responses to at least three parameters: charge difference across a transmembrane segment, its **total hydrophobicity**, and its hydrophobicity gradient. Relative signal strengths were estimated, and consequences for topol. prediction are discussed. Responses to transmembrane sequence may depend on **protein**-translocon interactions, but responses to charge difference may be mediated by the electrostatic field provided by anionic phospholipids.

ST transmembrane **protein** insertion orientation yeast; endoplasmic reticulum transmembrane **protein** insertion orientation

IT Membrane potential

(biol.; transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution)

IT Biological transport
 (intracellular; transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution)

IT **Proteins**, specific or class
 RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
 (membrane, integral, Type III; transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution)

IT Conformation
 (**protein**; transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution)

IT Electric charge
 Electrostatic force
 Endoplasmic reticulum
 Hydrophobic force
 Hydrophobicity
 Saccharomyces cerevisiae
 (transmembrane **protein** insertion orientation in yeast depends on the charge difference across transmembrane segments, their **total hydrophobicity**, and its distribution)

L8 ANSWER 5 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1997:270863 CAPLUS

DN 126:340121

TI The hydrophobic region of signal peptides is a determinant for SRP recognition and **protein** translocation across the ER membrane

AU Hatsuzawa, Kiyotaka; Tagaya, Mitsuo; Mizushima, Shoji

CS School Life Science, Tokyo University Pharmacy Life Science, Tokyo, 192-03, Japan

SO Journal of Biochemistry (Tokyo) (1997), 121(2), 270-277

CODEN: JOBIAO; ISSN: 0021-924X

PB Japanese Biochemical Society

DT Journal

LA English

RE.CNT 32 THERE ARE 32 CITED REFERENCES AVAILABLE FOR THIS RECORD
 ALL CITATIONS AVAILABLE IN THE RE FORMAT

TI The hydrophobic region of signal peptides is a determinant for SRP recognition and **protein** translocation across the ER membrane

AB Newly synthesized mammalian secretory **proteins** such as preprolactin are translocated across the endoplasmic reticulum (ER) in a signal recognition particle (SRP)-dependent manner. Recent studies revealed that there are two recognition steps for signal peptides during this translocation. The first step is recognition by SRP, which results in elongation arrest, and the second step is interaction between signal peptides and the translocation channel embedded in the ER membrane. To determine the roles of the hydrophobic region of signal peptides in the recognition by SRP and the membrane-embedded translocation machinery, we constructed chimeric **proteins** consisting of the mature region of preprolactin and signal peptides containing different nos. of leucine residues. The translocation of these chimeric **proteins** was completely dependent on SRP, and the efficiency increased as the number of leucine residues increased up to 10 and then decreased. Although the efficiency of elongation arrest also increased as the number of leucine residues increased up to 10, it only slightly decreased as the number increased up to 20. Similar results were obtained when the hydrophobic region was replaced by alternate leucine and alanine residues, except that the most efficient translocation occurred when the number was 14. Taken together, the present results suggest that the **total hydrophobicity** of the hydrophobic region of signal peptides is a determinant for recognition by both SRP and the membrane-embedded translocation machinery, although the specificities of the two signal recognition steps are slightly different from each other.

IT Ribonucleoproteins
 RL: BPR (Biological process); BSU (Biological study, unclassified); PRP (Properties); BIOL (Biological study); PROC (Process)
 (SRP (signal recognition particle); hydrophobic region of signal peptides is a determinant for SRP recognition and **protein** translocation across the ER membrane)

IT Hydrophobicity
 (hydrophobic region of signal peptides is a determinant for SRP recognition and **protein** translocation across the ER membrane)

IT Biological transport
 (intracellular; hydrophobic region of signal peptides is a determinant for SRP recognition and **protein** translocation across the ER membrane)

IT Endoplasmic reticulum
 (membrane; hydrophobic region of signal peptides is a determinant for SRP recognition and **protein** translocation across the ER membrane)

L8 ANSWER 6 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1996:483711 CAPLUS

DN 125:158761

TI High-performance liquid chromatography of fluorescent insulin derivatives

AU Petrochenko, E. V.; Kiselev, P. A.

CS Inst. Bioorg. Chem., Belaruss. Acad. Sci., Minsk, 220141, Belarus

SO Bioorganicheskaya Khimiya (1996), 22(3), 175-179

CODEN: BIKHD7; ISSN: 0132-3423

PB MAIK Nauka

DT Journal

LA Russian

AB The reversed-phase HPLC of porcine insulin modified by fluorescent labeling with dansyl chloride, fluorescein isothiocyanate, and an N-hydroxysuccinimide ester of 3-carboxyl derivative of Nile Red was studied. Mono-, di-, and tri-Dns-insulins (substituted at residues Gly1 of the A-chain and Phe1 and Lys29 of the B-chain), as well as isomeric 5'- and 6'-fluoresceinthiocarbamoyl-Phe1 insulin derivs. were separated on the anal. and semipreparative scale. The results were interpreted in terms of conservation of the globular structure in the modified **proteins** and their surface-mediated interaction with the reversed-phase sorbent. Observed retention times correlated with the **total hydrophobicity** of the surface region containing the incorporated label (in the case of monosubstituted derivs.) or with the **total hydrophobicity** of chromatog. contact regions located between labels (in the case of di- and trisubstituted derivs.).

L8 ANSWER 7 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1995:404737 CAPLUS

DN 122:182868

TI Comparison of the potential membrane insertion geometries of Escherichia

coli low molecular weight penicillin binding **protein** anchors

AU Roberts, Martin G.; Phoenix, David A.

CS Department of Mathematics and Statistics, Univ. of Central Lancashire, Preston, PR1 2HE, UK

SO Biochemical Society Transactions (1995), 23(1), 33S

CODEN: BCSTB5; ISSN: 0300-5127

PB Portland Press

DT Journal

LA English

TI Comparison of the potential membrane insertion geometries of Escherichia coli low molecular weight penicillin binding **protein** anchors

AB The anchor characteristics of low-mol.-weight penicillin-binding **proteins** were investigated as full 3-dimensional geometries. Software was developed to explore a discrete set of membrane insertion geometries. The **total hydrophobicity** inserted into the membrane and the maximum depth of penetration were used as parameters to estimate the strength of anchoring. The anal. indicated that PBP5 and PBP6, less strongly, interact with the membrane, but that PBP4 attaches loosely, if at all. These results agree with exptl. data.

ST **protein** penicillin binding membrane anchoring Escherichia

IT Simulation and Modeling, biological
 (of potential membrane insertion geometries of Escherichia coli
 low-mol.-weight penicillin-binding **protein** anchors)

IT Cell membrane
 Escherichia coli
 (potential membrane insertion geometries of Escherichia coli
 low-mol.-weight penicillin-binding **protein** anchors)

IT **Proteins**, specific or class
 RL: BSU (Biological study, unclassified); BIOL (Biological study)
 (PBP (penicillin-binding **protein**), potential membrane
 insertion geometries of Escherichia coli low-mol.-weight
 penicillin-binding **protein** anchors)

L8 ANSWER 8 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1993:58316 CAPLUS
 DN 118:58316

TI Heat-related changes to the hydrophobicity of cheese whey correlate with
 levels of native β -lactoglobulin and α -lactalbumin

AU Regester, Geoffrey O.; Pearce, R. John; Lee, Victor W. K.; Mangino,
 Michael E.

CS Div. Food Process., CSIRO, Highett, 3194, Australia

SO Journal of Dairy Research (1992), 59(4), 527-32
 CODEN: JDRSAN; ISSN: 0022-0299

DT Journal

LA English

AB Correlations were identified between levels of the native whey
proteins, β -lactoglobulin and α -lactalbumin and the
 surface and **total hydrophobicities** of cheese whey in
 response to different heat treatments. Heat-induced changes in the native
 β -lactoglobulin content and surface hydrophobicity of whey exhibited
 the most significant linear relationship while correlations between
total hydrophobicity and the native **proteins**
 were less significant because of an atypical rise in the n-heptane-binding
 capacity of whey after high-temperature treatment. The content of native
 β -lactoglobulin in whey was more sensitive to heating than was the
 content of native α -lactalbumin, while heat-related changes in the
total hydrophobicity of whey were generally greater than
 similar changes in surface hydrophobicity.

L8 ANSWER 9 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1992:168466 CAPLUS
 DN 116:168466

TI Effects of **total hydrophobicity** and length of the
 hydrophobic domain of a signal peptide on in vitro translocation
 efficiency

AU Hikita, Chinami; Mizushima, Shoji

CS Inst. Appl. Microbiol., Univ. Tokyo, Tokyo, 113, Japan

SO Journal of Biological Chemistry (1992), 267(7), 4882-8
 CODEN: JBCHA3; ISSN: 0021-9258

DT Journal

LA English

TI Effects of **total hydrophobicity** and length of the
 hydrophobic domain of a signal peptide on in vitro translocation
 efficiency

AB The hydrophobic domain of a signal peptide of OmpF-Lpp, a model secretory
protein, was systematically engineered so as to be composed of
 different lengths of polyleucine residues or polymers with alternate
 leucine and alanine residues, and the effects of the length and nature of
 the hydrophobic stretch on the rate of in vitro translocation were studied
 using everted membrane vesicles of Escherichia coli. The translocation
 reaction exhibited high substrate specificity as to the number of hydrophobic
 residues. The results suggest that the hydrophobic domain is recognized
 specifically by a component(s) of the secretory machinery rather than
 nonspecifically by the hydrophobic region of the membrane. The in vitro
 translocation thus demonstrated required SecA and ATP and was markedly
 enhanced upon imposition of the protonmotive force, as in the case of
 secretory **proteins** possessing a natural signal peptide. The
 highest translocation rate was obtained with the octamer in the case of

polyleucine-containing signal peptides, whereas it was the decamer in the case of ones contained both leucine and alanine. These results suggest that the **total hydrophobicity** of the hydrophobic region of the signal peptides is an important determinant of the substrate specificity.

ST signal peptide hydrophobicity length **protein** secretion
IT Hydrophobicity
(of signal peptides, **protein** secretion efficiency in Escherichia coli dependence on)
IT Escherichia coli
(**protein** secretion by, signal peptide hydrophobicity and length effect on efficiency of)
IT **Proteins**, specific or class
RL: BIOL (Biological study)
(gene secA, **protein** secretion by Escherichia coli dependence on, signal peptide hydrophobicity in length in relation to)
IT Force
(protonmotive, **protein** secretion by Escherichia coli dependence on, signal peptide hydrophobicity in length in relation to)
IT Biological transport
(secretion, of **proteins**, by Escherichia coli, signal peptide hydrophobicity and length role in)
IT **Proteins**, specific or class
RL: BIOL (Biological study)
(secretory, secretion of, by Escherichia coli, signal peptide hydrophobicity and length effect on efficiency of)
IT Peptides, properties
RL: PRP (Properties)
(signal, hydrophobicity and length of, **protein** secretion by Escherichia coli dependence on)
IT 7732-18-5
RL: BIOL (Biological study)
(hydrophobicity, of signal peptides, **protein** secretion efficiency in Escherichia coli dependence on)
IT 56-65-5, 5'-ATP, biological studies
RL: BIOL (Biological study)
(**protein** secretion by Escherichia coli dependence on, signal peptide hydrophobicity and length in relation to)

L8 ANSWER 10 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1987:98738 CAPLUS
DN 106:98738
TI High-performance liquid-chromatographic properties of peptides and **proteins** on a dihydroxyalkyl-bonded silica stationary phase
AU Meyerson, Laurence R.; Abraham, Kakkudiyil I.
CS Dep. Chem. Pharmacol., Am. Cyanamid Co., Mahwah, NJ, 07430, USA
SO Peptides (New York, NY, United States) (1986), 7(3), 481-9
CODEN: PPTDD5; ISSN: 0196-9781
DT Journal
LA English
TI High-performance liquid-chromatographic properties of peptides and **proteins** on a dihydroxyalkyl-bonded silica stationary phase
AB The chromatog. behavior of biol. relevant peptides and **proteins** in the mol. weight range 200-200,000 dalton units were studied on a size exclusion matrix column consisting of an aqueous compatible dihydroxyalkyl bonded silica support. The mechanism of separation was dependent on hydrodynamic radius, hydrophobic and ionic interactions. Support for this contention is based on the chromatog. properties of these peptides and **proteins** at different mobile phase ionic strengths and pH, oxidation state of amino acid residues and **total hydrophobicity** of the peptide or **protein**. This column is also capable of separating native angiotensin I from its iodinated congener. Recoveries of **proteins** and peptides from this column ranged 70-100%. Unlike typical reversed phase sepns., this modified silica chromatog. media allows for an alternative technique employing aqueous eluents for rapid separation/isolation and purification of peptides and **proteins** from natural or synthetic sources.
ST HPLC peptide **protein** dihydroxyalkyl silica; liq chromatog

peptide **protein**
IT Albumins, analysis
Myoglobins
Ovalbumins
Peptides, analysis
Proteins, analysis
RL: ANT (Analyte); ANST (Analytical study)
(chromatog. of, high-performance liquid, on dihydroxy-alkyl bonded silica)

IT Chromatography, column and liquid
(high-performance, of peptides and **proteins**, on dihydroxyalkyl-bonded silica)

IT 105845-15-6
RL: ANST (Analytical study)
(peptides and **protein** separation by HPLC on)

L8 ANSWER 11 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1983:419193 CAPLUS
DN 99:19193
TI Characteristics of **protein**-aqueous medium interactions measured by partition in aqueous Ficoll-Dextran biphasic system
AU Zaslavskii, B. Yu.; Mestechkina, N. M.; Rogozhin, S. V.
CS Inst. Elementoorg. Compd., Moscow, 117813, USSR
SO Journal of Chromatography (1983), 260(2), 329-36
CODEN: JOCRAM; ISSN: 0021-9673
DT Journal
LA English
TI Characteristics of **protein**-aqueous medium interactions measured by partition in aqueous Ficoll-Dextran biphasic system

AB Partitioning of a number of **proteins** in the aqueous Ficoll-400-Dextran-70 biphasic system was studied at pH 7.4 under varied ionic compns. The relative hydrophobicities of the **proteins** were estimated, and the contributions of the interactions of the ionogenic and nonionic groups of a **protein** with an aqueous environment to the **total hydrophobicity** of the **protein** were evaluated. Some arguments in support of the biol. significance of the effect of ionic composition on the relative hydrophobicity of biol. macromols. are given. Possible applications of the partition technique to **protein** research are discussed.

ST **protein** partition Ficoll dextran system; hydrophobicity
protein partition

IT Partition
(of **proteins**, in aqueous Ficoll-dextran biphasic system, hydrophobicity in relation to)

IT Hydrophobicity
(of **proteins**, partition in aqueous Ficoll-dextran biphasic system in relation to)

IT Ferritins
Myoglobins
Ovalbumins
Proteins
RL: PRP (Properties)
(partition of, in aqueous Ficoll-dextran biphasic system, hydrophobicity in relation to)

L8 ANSWER 12 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
AN 1977:595842 CAPLUS
DN 87:195842
TI Conformation of **proteins**: hydrophobic ordering of strands in β -pleated sheets
AU Sternberg, M. J. E.; Thornton, J. M.
CS Lab. Mol. Biophys., Dep. Zool., Oxford, UK
SO Journal of Molecular Biology (1977), 115(1), 1-17
CODEN: JMOBAK; ISSN: 0022-2836
DT Journal
LA English
TI Conformation of **proteins**: hydrophobic ordering of strands in β -pleated sheets

AB The influence of hydrophobic free energy on strand order in β -pleated sheets was studied. A hydrophobic free energy was assigned to each type of amino acid and the **total hydrophobicity** of each strand in a sheet was calculated by summing the energies for all residues in that strand. In 30 of the 39 sheets studied, there is evidence that the strands with greatest hydrophobic potential tend to occur in the center of the sheet, whereas the more hydrophilic strands occupy the edge positions in the sheet. In 20 of the 30 sheets, the most hydrophobic strand is buried and the remaining strands are arranged in order of decreasing hydrophobicity outwards in both directions. The **total hydrophobicity** of a strand reflects not only the amino acid composition of the strand, but also its length. Longer strands are potentially more hydrophobic and occur most frequently in the center of the sheet. This suggests that hydrophobic ordering is one important factor in determining strand order, possibly reflecting hydrophobic nucleation. In addition, the **total hydrophobicities** of opposite sides of the sheets were calculated. There is a good correlation between the observed relative exposure to solvent and the calculated hydrophobicities. These observations underline the importance of hydrophobic free energy in determining the tertiary structure of the **protein**.

ST **protein** conformation hydrophobic ordering
IT **Proteins**
RL: PRP (Properties)
(conformation of, hydrophobic ordering of β -structure in)

IT Chains, chemical
(conformation of, of **proteins**, hydrophobic ordering of β structure in)

IT Hydrophobicity
(in **protein** β -structure ordering)

IT Free energy
(of hydrophobicity, in **protein** β -structure ordering)

IT **Proteins**
RL: PRP (Properties)
(iron, conformation of, hydrophobic ordering of β structure in)

L8 ANSWER 13 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN

AN 1970:421379 CAPLUS

DN 73:21379

TI Correlations between the amino acid sequence and conformation of immunoglobulin polypeptide chains

AU Welscher, H. D.

CS World Health Org. Int. Ref. Centre Immunoglobulins, Lausanne, Switz.

SO Behringwerk-Mitteilungen (1969), 49, 133-42

CODEN: BEHRAP; ISSN: 0067-4885

DT Journal

LA English

AB The influence of nonpolar amino acid residues on the tertiary structure of immunoglobulin light chains was considered in terms of hydrophobic interactions, and of the stereochem. arrangement of hydrophobic residues in the primary structure. The hydrophobicities (C. J. Tanford, 1962) of light chains were calculated. In γ -type Bence-Jones **protein** New, 110 of 216 residues were nonpolar and a **total hydrophobicity** of 219 kcal or 1010 cal/residue were calculated. The fractional charge on the mol. (= total charge at physiol. pH/total number of residues) was 0.17 units/residue. Fifteen other light chains of known sequence had hydrophobicities near 1000 cal/residue, and fractional charges near 0.19 units/residue, despite high sequence variability. It was calculated that the entropy and enthalpy terms contributing to the free energy difference between the unfolded and native conformations of polypeptide chains were approx. equal for **proteins** containing no SS bridges, but unequal in **proteins** containing SS bridges. The discrepancy was greater in RNase which has a dependently looped structure than in light chains where the SS occur in independent loops. The pattern of distribution of nonpolar residues along the chains was common to 15 individual light chains. There were 63 identical sequence sites (30 in the variable, 33 in the constant regions) consistently occupied by nonpolar residues. Polar residues showed no characteristic pattern. It was considered to be essential for proper globular folding of the molecule

that certain invariant (nonpolar) regions be present, so that noncovalent interactions would result in a minimization of the conformational free energy. Only a well-defined pattern in the primary sequence would allow for this specific globular folding.

ST immunoglobulin polypeptides thermodyn; polypeptides immunoglobulin thermodyn; thermodyn immunoglobulin polypeptides; **proteins** conformation thermodyn

IT **Proteins**
 RL: BIOL (Biological study)
 (Bence-Jones, conformation of, amino acid sequence in relation to)

IT Potential barriers
 (rotational, of **proteins**, hydrophobic amino acid residues in relation to minimization of)

L8 ANSWER 14 OF 14 CAPLUS COPYRIGHT 2005 ACS on STN
 AN 1970:86387 CAPLUS
 DN 72:86387
 TI Correlations between amino acids sequence and conformation of immunoglobulin light chains. I. Hydrophobicity and fractional charge
 AU Welscher, H. D.
 CS Inst. Biochem., Univ. Lausanne, Lausanne, Switz.
 SO International Journal of Protein Research (1969), 1(4), 253-65
 CODEN: IPRRBQ; ISSN: 0020-7551
 DT Journal
 LA English
 AB The significance of nonpolar and of charged residues for the conformation of light chains is discussed, based on the amino acid sequence of 15 light chains and on the amino acid composition of light chains from 11 species. The nonpolar residues contribute to the conformational stability by hydrophobic interactions with an average hydrophobicity of .apprx.1000 cal/residue; this value is essentially independent of isotypic and idiotypic sequence variability, and is similar to that for other globular **proteins**. While the **total hydrophobicity** of many globular **proteins** containing no SS bridges compensates almost exclusively for their conformation entropy, a significant discrepancy is observed in the case of light chains. This may reflect the loss of conformational entropy due to the 2 SS bridges forming independent covalent loops. The ionized residues give a fractional charge close to 0.20 units/residue. This relatively low value, together with the relatively high average hydrophobicity, explains qual. many of the association and thermal properties of light chains. Variable and constant regions of light chains exhibit nearly identical average hydrophobicities and fractional charges, suggesting that the mols. are folded into 2 distinct structural subunits of compact conformation. Some preliminary results on heavy chains are also considered. The fractional charges of the Fd fragments are much lower than those of the Fc fragments. This may facilitate the intimate contact of the light chain with the former fragment in the intact antibody mol.